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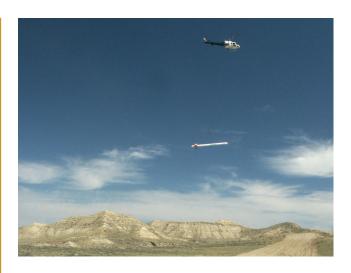
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ON THE COVER

TEM (Transmission Electron Microscopy) superlattice Darkfield image of gamma prime precipitates in one of the nickel-based superalloys currently being studied for GE evaluation.



newlognews is a quarterly newsletter, which highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula turner@netl.doe.gov. or call 541-967-5966.

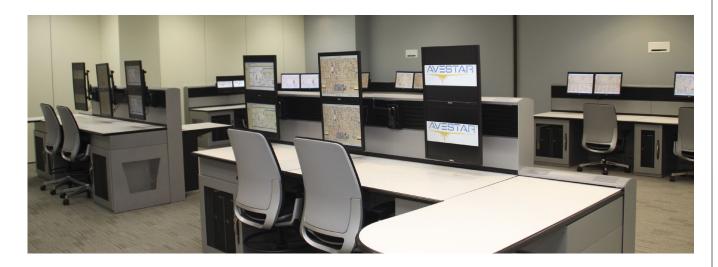


Helicopter Electromagnetic Surveys Locate Potential Hazards at Coal Waste Impoundments

NETL researchers and collaborators from the University of Pittsburgh evaluated helicopter electromagnetic (HEM) surveys from 14 coal waste impoundments in West Virginia. The researchers found that HEM surveys could accurately locate water saturated zones within the embankments (dams) and thereby identify failure-prone areas. Currently, the location and elevation of water-saturated zones are determined by installing piezometers, a process required by the Department of Labor, Mine Safety and Health Administration (MSHA). However, this process is expensive, labor intensive, and provides information only near the location of the piezometers.

In contrast, HEM surveys can rapidly provide the same information for an entire impoundment, including areas where it would be impossible to install piezometers. HEM surveys can also identify areas of unconsolidated slurry that are buried beneath multiple, thick lifts of coarse coal waste, an unstable condition that can lead to solifluction (soil fluction, a type of mass wasting where waterlogged sediment moves slowly downslope over impermeable material) and rapid, catastrophic dam failure. Findings from this research suggest that HEM might be useful for locating failure prone areas in dams surrounding coal ash impoundments too. This research has been published in the latest issue of *Geophysics* (Vol. 75, No. 6).

Contact: Richard Hammack, 412-386-6585



NETL Center Completes Site Acceptance Test for IGCC Dynamic Simulator

Final site acceptance testing was completed for an integrated gasification combined cycle (IGCC) dynamic simulator deployed at NETL's Advanced Virtual Energy Simulation Training and Research (AVESTAR™) Center.

Developed as a part of NETL's initiative to advance new clean coal technology, the AVESTAR™ Center is focused on training engineers and energy plant operators in the efficient, productive, and safe operation of highly efficient power generation systems that also protect the environment.

Targeted to energy and process, engineering and construction, and technology supply industries, the AVESTAR Center aims to develop a workforce well-prepared to operate, control, and manage next-generation power plants with carbon capture. The Center also promotes NETL's outreach mission by offering hands-on simulator training and education to researchers and university students. Current training and research objectives will help meet aggressive NETL program goals for advanced IGCC power stations capable of 90 percent pre-combustion CO₂ capture, as well as low sulfur, mercury, and NO₂ emissions.

The AVESTAR Center offers the full-scope, high-fidelity, real-time dynamic simulator with operator training system (OTS) capabilities for a commercial-scale IGCC plant with CO₂ capture and compression. The simulator builds on, and reaches beyond, existing combined-cycle and conventional-coal power plant simulators to combine, for the first time, a "gasification with CO₂ capture" process simulator with a "combined-cycle" power simulator together in a single dynamic simulation framework.

NETL planned, developed, tested, and deployed the IGCC dynamic simulator in collaboration with energy experts from West Virginia University, Fossil Consulting Services, Invensys Operations Management, and other industry and university partners. AVESTAR's IGCC training programs are projected to be up and running in May 2011 at state-of-theart simulation facilities located at NETL in Morgantown, WV, and at West Virginia University's National Research Center for Coal and Energy. Looking forward, NETL will continue to build AVESTAR's portfolio of dynamic simulators, immersive training systems, and advanced research capabilities to satisfy industry's growing need for training and experience with the operation and control of high-efficiency, near-zero emission energy plants.

Contact: Stephen E. Zitney, 304-285-1379



NETL's walk-in freezer at the NETL-OSU Repository for Sediment Cores from Natural Gas Hydrate Systems' at OSU's Marine Geology Repository.



Cores in "D-tubes' stored in the Repository.

New Repository for Natural Gas Hydrate Sediment Cores Opens

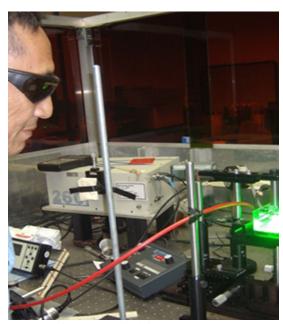
Since 2005, the National Methane Hydrate R&D Program at NETL has been heavily involved in coring expeditions in support of natural gas hydrate research worldwide. The collected cores provide priceless geologic, physical properties, and geochemical information critical to research conducted by field scientists, experimentalists, and modelers. However, access to these unique cores by the research community has been limited and uncoordinated, and the cores have been subject to loss or destruction due to inadequate storage conditions.

To ensure the integrity of these samples and data, a unique facility has been established by NETL in conjunction with Oregon State University at its College of Oceanic and Atmospheric Sciences' Marine Geology Repository (MGR). The last steps in finalizing the establishment of the NETL-OSU Repository for Sediment Cores from Natural Gas Hydrate Systems occurred last week with the installation of a large -10 °F walk-in freezer at the MGR and a -86 °C ultra-low temperature freezer on the OSU campus. The addition of the two freezers by NETL expands the Repository's storage capabilities to include samples and cores that must remain frozen for preservation. The MGR facilities are well-equipped for long-term maintenance

and management of thousands of geologic samples and refrigerated sediment cores. In addition, the OSU curators will ensure improved access to the natural gas hydrate sediment cores for sampling and analysis.

Refrigerated cores from the 2005 Gulf of Mexico Gas Hydrate JIP Leg I expedition are now stored at the Repository and frozen cores from the BP-DOE Alaska North Slope Mount Elbert are being transported from Anchorage to the Oregon site. In addition, samples from the recent expedition with South Korea in the East Sea were sent to OSU for microbiologic analyses and are now housed in the -86 °C freezer. The NETL-OSU Repository is a critical step in establishing a core legacy that will aid natural gas hydrate research for generations to come and will aid research on the impact of gas hydrates on climate change, earth systems, and energy production potential.

Contact: Kelly Rose, 541-967-5883



NETL's Dr. Phuoc Tran in his laboratory.

Nanoparticle Production Method Focuses on Cancer Treatment

An NETL scientist has developed a method of producing novel, *non-toxic* gold nanoparticles for cancer treatment and targeted drug delivery to replace the potentially toxic nanoparticles typically produced by current chemical methods. The process involves only water, two lasers, and a piece of gold, and has no toxic chemicals.

When green and infrared lasers strike the surface of a thin gold foil, gold nanoparticles are gouged from the surface in a process called laser ablation. The nanoparticles bunch together in water due to the surface forces, just as nanoparticles produced by standard chemical methods do. The individual nanoparticles must be "unbunched" to be injected into the human body. Standard practice has been to use a toxic surfactant to separate the particles, but this method uses corn starch, potato starch, or chitosan, a natural product from shellfish.

Besides helping to separate the clumps of gold nanoparticles, this method also uses these natural products to try to control the size and shape of the

nanoparticles. The gold particles initially produced by laser ablation are usually spherical, but gold cylinders called nanorods would be preferable. Typically, during clinical treatment, gold nanoparticles are injected into a tumor and then irradiated with infrared light, which can penetrate layers of the patient's skin. The light heats up the gold and causes it to destroy nearby cancerous cells, but only if the nanoparticles are of the right size and shape to absorb the light. Spherical nanoparticles will not work. It takes gold nanorods with precisely the right length and diameter to interact with the infrared light, causing surface electrons to vibrate and heat up to destroy the cancer cells. Research continues to control laser parameters, the concentration of the natural substances, and the temperature and the mixing duration to control shape and size of the gold nanoparticles.

(Click here to read more about these nanoparticles.)

Contact: Phuoc Tran, 412/386-6024

NETL, NIST Collaboration Uses Neutrons to Study CO₂ Sorbents

Scientists from NETL and the U.S. Department of Commerce's National Institute of Standards and Technology (NIST) have been collaborating to determine how structurally dynamic sorbents rearrange their atoms to selectively adsorb CO_2 from mixed gas streams containing CH_4 and N_2 . The NETL-NIST team has used neutron diffraction and neutron vibrational spectroscopy to determine changes that occur in the positions and motions of atoms when CO_2 is absorbed by a structurally dynamic metal organic framework (MOF) sorbent. A third technique, called small angle neutron scattering, was used to study how the sorbent particle's size, shape, and packing density changed as a result of these atomic-level structural changes.

The advantage of using neutrons for studying CO₂ capture sorbents is that they can nondestructively penetrate matter in a manner that cannot be accomplished with X-rays or other techniques. In this regard, neutron methods are truly in situ, allowing researchers to investigate the positions, motions, and energetics of atoms in these sorbents at elevated temperatures and pressures. Early data analysis points to a "breathing" motion between atomic sheets in the sorbent, which is initiated specifically by the CO₂ molecule in mixed streams containing N₂, CH₄, and other gases. This atomic level breathing motion causes the macroscopic size of the sorbent particles to increase by up to 50 percent, thus illustrating a link between atomic scale-phase transitions and more practical engineering considerations such as particle morphology and sorbent bed packing density.

An unusual behavior was noted when the sorbents released the CO₂, involving a complex, multiphase, sorbent structure unique to the desorption process. This observation helps explain a well-known desorption hysteresis noted in the isotherms of these MOFs. Understanding this hysteresis will enable engineers to design improved pressure swing adsorption cycles for these sorbents.

Contact: Christopher Matranga, 412-386-4114

NETL, NASA Collaborate on Extreme Temperature Thermal Barrier Coatings

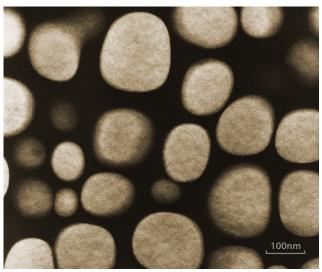
NETL, in collaboration with the National Aeronautics and Space Administration (NASA), recently completed the first qualification testing of an extreme temperature composite architecture that is being developed for advanced hydrogen-fired turbine applications. This testing was done using a nickel-based single crystal René N5 substrate material, NETL's Coatings for Industry's (CFI) A1D bond coat system, a commercially applied state-of-the-art air plasma sprayer, a yttria-stabilized zirconia layer, and NASA's extreme temperature overlayer.

Laser thermal flux testing was conducted at NASA where the external surface temperatures of the overlayer reached about 1480 °C, while the bond coat interface temperature was maintained at about 1120 °C through back-side cooling of the test coupon. The test coupon was exposed to 50 thermal transitions wherein the composite architecture was heated for one hour, and subsequently cooled to room temperature in 3 minutes under cyclic test conditions. The coating was adherent and intact after completion of the cyclic qualification test. Future testing is planned to demonstrate the impact of steam, as well as the inclusion of diffusion barrier coatings on the composite thermal barrier coating architecture.

Contact: Mary Anne Alvin, 412-386-5498



One of the cast Ni-alloy plates for welding trials is shown above.



TEM (Transmission Electron Microscopy) superlattice Darkfield image of gamma prime precipitates in one of the nickel-based superalloys currently being studied.

Experimental Ni-Based Superalloy Samples for Advanced Steam Turbine Applications

NETL recently provided GE, an advanced ultra supercritical (A-USC) consortium team member, with multiple cast versions of traditionally wrought Ni-based superalloys for evaluation. The samples were created using a casting technique and an optimized homogenization heat treatment developed by NETL (patent pending). NETL has been working towards improving the efficiency of coal-fired power plants for a number of years. A core enabler to this goal is increasing the operating temperature of the power plant. High-temperature components within conventional coal-fired power plants are manufactured from ferritic/martensitic steels, but the proposed steam temperature in the A USC power plant (760 °C) is too high for ferritic/martensitic steels; thus, Ni-based superalloys are being considered.

By working with GE, NETL is better able to determine the suitability of these materials for advanced steam turbine applications, such as valve bodies and turbine casings, which are too complex for wrought component manufacturing techniques. The castings are being evaluated for microstructure, weldability, and mechanical performance, including strength and creep resistance.

Contacts: Paul Jablonski, 541-967-5982; Christopher Cowen, 541-967-5952; and Edward Argetsinger, 541-967-5870





Steel bars bonded with the new adhesive over an area of 1 square inch were able to suspend more than 200 pounds without separating

Researchers Use CO₂ to Create Adhesives

Researchers are incorporating CO₂ into polymeric materials similar to epoxy. Like epoxy, these materials are made by mixing two liquid components: a multifunctional cyclic carbonate and a multi-functional amine. These components react to form a cross-linked poly (hydroxyurethane) that is strong and adheres well to aluminum and glass surfaces. In addition to their use as adhesives, these materials also have potential application as sealants and binders for composites such as fiberglass and plywood. The CO₃ is incorporated into the polymeric materials through the multi-functional cyclic carbonates. Using novel chemistry, the CO₂ is combined with inexpensive reagents to form the liquid precursor. Developing technology that utilizes CO₂ as a chemical feedstock in the preparation of useful materials will both reduce the quantity of the greenhouse gas that must be geologically sequestered and allow industry to partially offset sequestration costs through sales of these materials.

Contact: Dave Luebke, 412-386-4118

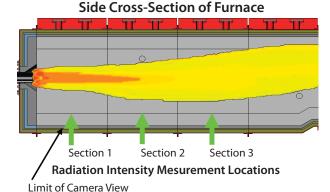
IGCC Optimization Approach Enhances Efficiency, Flexibility

Researchers at NETL and West Virginia University have developed a three-phase, top-down, optimization-based approach for designing integrated gasification combined cycle (IGCC) plants with pre-combustion CO₂ capture in a process simulator environment.

In the first phase, important global design decisions are made on the basis of plant-wide optimization studies with the aim of increasing IGCC thermal efficiency and thereby making better use of coal resources while reducing CO₂ emissions. For an IGCC plant with 90 percent CO₂ capture, the optimal combination of the extent of carbon monoxide conversion in the water-gas shift (WGS) reactors and the extent of CO₂ capture in the SELEXOL solvent process is determined in this first design phase. In the second design phase, the impact of local decisions for the CO₂ capture and Claus sulfur units is explored considering the optimum values of the decision variables from the first phase as additional constraints. In the third design phase, the operating conditions are optimized considering the optimum values of the decision variables from the first and second phases as additional constraints.

The operational flexibility of the IGCC plant must be taken into account before making final design decisions. Two studies were conducted on the operational flexibility of WGS reactors while one study focused on the operational flexibility of the sour water stripper. At the end of the first iteration, after executing all the phases once, the net plant efficiency (HHV basis) increased to 34.1 percent compared to 32.5 percent in a previously published report (DOE/NETL-2007/1281). This study shows that the three-phase, top-down design process simulator approach is potentially very useful for improving efficiency and flexibility of IGCC power plants with CO₂ capture. In addition, the study identifies a number of key design variables that strongly affect the efficiency of an IGCC plant with CO₂ capture. A paper titled "Steady-State Simulation and Optimization of an Integrated Gasification Combined-Cycle Power Plant with CO₂ Capture," which describes these latest optimization advances, was recently published in the peer-reviewed journal, Industrial & Engineering Chemistry Research.

Contact: Stephen E. Zitney, 304-285-1379



NETL Researchers Demonstrate New Approach to Manipulate Thermal Radiation

NETL researchers have completed their analysis of thermal radiation data collected during pilot-scale oxy-fuel experiments at the University of Utah's 3.5 Mbtu/hr pulverized coal furnace. The researchers found that the thermal radiation from the flame can be significantly boosted by injecting some of the oxygen within the fuel-carrying gas-stream into the near-burner combustion zone as opposed to blending all of it into the flue gas recirculation stream preburner. Thus, modifying oxygen injection strategy at the burner provides a new degree of freedom in manipulating the flame's radiant heat flux. This is a significant step in making an oxy-coal retrofit feasible.

The experiments consisted of parametric testing of an oxy-fuel burner developed by Siemens and Reaction Engineering International. Various strategies for oxy-firing were examined in the context of retrofitting a conventional facility and air-firing data were collected for comparison. The thermal radiation profile from the flame, measured using a series of total radiometers calibrated for this purpose by NETL researchers, is of particular interest because one of the challenges of an oxy-fuel retrofit is overcoming or minimizing the changes in heat transfer throughout the system. Further investigation is needed to quantify how oxygen jets impact flame morphology so that localized radiant heat transfer effects within a boiler can be predicted. The results will appear in an upcoming International Energy Agency Greenhouse Gas R&D Programmed special oxy-fuel publication.

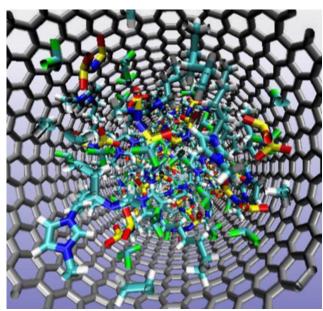
Tests Completed on Novel Low-Emission Fuel Injector

Testing of a novel low-emission hydrogen diffusion flame injector for hydrogen gas turbine applications has been completed in NETL's high pressure combustion facility. Based on prior laboratory-scale studies of hydrogen dilute diffusion flames, the injector design was optimized to use a dense array of small diameter jets. These jets provided a high-velocity, nitrogen-diluted hydrogen fuel flow to the combustor to reduce NO_{x} emissions at realistic firing rates. The NO_{x} reduction results from the fact that multiple discrete, compact, highly strained diffusion "flamelets" are produced with this design, which enables fast quenching of combustion temperatures.

Stable operation of the injector was demonstrated at pressures of 4-16 atm and with fuel jet velocities of 100-300 m/s. NO $_{\rm x}$ emissions were observed to vary with combustor pressure, fuel jet velocity, and diluent concentration. NO $_{\rm x}$ emissions of 4-6 ppmv (at 15 percent exhaust O $_{\rm 2}$) were achieved at 16 atm with flame temperatures of 1600-1900K and 50 percent nitrogen dilution. The full results are described in a paper which has been submitted to the ASME-IGTI Turbo Expo 2011.

Contact: Nathan Weiland, 412-386-4649

Contact: Danylo Oryshchyn, 541-967-5865

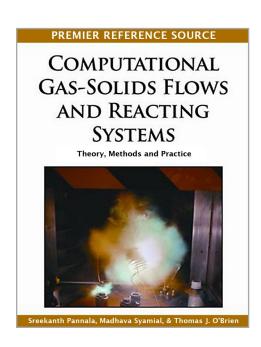


A snap shot for ionic liquid [hmim][Tf2N] confined in the (20,20) carbon nanotubes from molecular simulations.

Review Published of *In-Situ*Electromagnetic Techniques for Oil Shale Processing

Researchers Alexandra Hakala, Sheila Hedges, and Yee Soong, in collaboration with University of Pittsburgh Professor William Stanchina, recently published a critical review on the dielectric properties and electromagnetic heating of Green River Formation oil shales. Electromagnetic techniques are of interest because the applied energy can selectively detect and heat organic layers present within oil shale. The review, which was published in the journal *Fuel Processing Technology*, presents and synthesizes prior work on the influence of applied frequency, oil shale grade, water, and temperature on the dielectric properties of oil shales and can aid the future development of frequency- and temperature-specific *in-situ* retorting technologies and oil shale grade assay tools.

Contact: Alexandra Hakala, 412-386-5487



New Book Published on Computational Gas-solids Flows

A book entitled Computational Gas-Solids Flows and Reacting Systems: Theory, Methods, and Practice, edited by Sreekanth Pannala (ORNL) and NETL scientists Madhava Syamlal and Thomas J. O'Brien, was published by Engineering Science Reference, Hershey, PA. This collection of 13 chapters on gas-solids flow describes the new theories, numerical methods, and applications that have emerged during the last two decades. Syamlal and Pannala wrote the chapter entitled "Multiphase continuum formulation for gas-solids reacting flows," and NETL scientist Ronald W. Breault wrote the chapter entitled "Mass and heat transfer modeling."

Contact: Madhava Syamlal, 304-285-4685

New Structures Discovered in Carbon Nanotube Hybrid Systems

Theoretical studies performed on ionic liquids (ILs) confined within carbon nanotubes (CNT) have discovered the presence of nano-scale ordering, which has profound implications for the gas transport properties of the system. In the systems studied, more cations are located close to the tube wall while more anions are located in the tube center. This arrangement, which differs markedly from the random distribution present in the bulk IL, changes the interactions of the system with mixtures of CO₂ and H₂. The composite material exhibits higher sorption selectivity for CO, over H₂ than either the IL or the CNT, leading to improved capture solvent properties in the hybrid. Even more interesting, the composite appears to slow H₂ molecular diffusion to only 1.5 times that of CO₂. In contrast, H₂ diffuses about 10 times faster than CO₂ in the bulk IL. This greater relative rate of CO₂ transport may allow membrane researchers to improve the selectivity and flux of membranes made of composite materials for CO₃ capture applications. This work was recently published in the Journal of Physical Chemistry B, 2010, 114, pp 15029-15041.

Contact: Wei Shi, Dave Luebke, 412-386-4118

Researchers Publish Chapter on Materials Challenges in Renewable, Alternative Energy

NETL researchers recently published a chapter in the Wiley book series Ceramic Transactions (Vol. 224, 2011, pp. 377-385). The chapter, "Addressing the Materials Challenges in Converting Biomass to Energy," discusses the use of biomass and coal mixtures in next generation materials and fuels conversion technologies, emergent material compatibility issues in gasification refractory development, contaminant effects on Fischer-Tropsch (F-T) fuel production technology, and the efficient treatment of light F-T off-gases using CO₂ reforming and recycle of pre-combustion capture CO₂.

Contact: Todd Gardner, 304-285-4226 and James Bennett, 541-967-5983

Synchrotron X-rays Shine Light on the Reactivity of Water-Gas Shift Catalysts

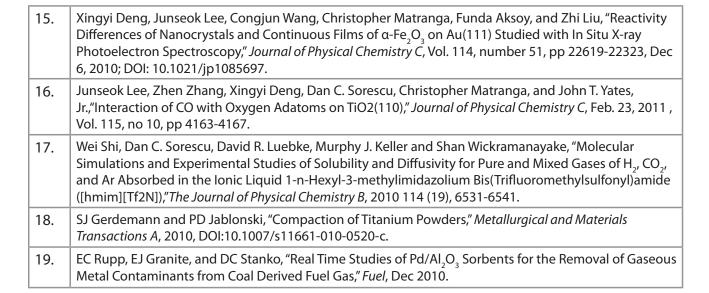
To better understand how water-gas shift (WGS) catalysts convert carbon monoxide and water from gasified coal into valuable fuels, such as hydrogen, researchers at NETL have turned to synchrotron based X-ray techniques. Synchrotron X-rays are a billion times brighter than the sun and are bright enough to produce results on catalyst systems in a matter of hours, whereas lower intensity laboratory based X-ray techniques would take almost a decade to produce the same data.

NETL researchers recently reported on their use of synchrotron X-rays for studying an iron-based WGS catalyst in the Journal of Physical Chemistry C (Vol. 114, 2010, pp 22619-22623). In this work, they used a specialized technique called ambient pressure X-ray photoelectron spectroscopy to determine the mechanism of the catalytic reaction, the molecular intermediates involved, and the electronic structure changes required to activate these catalysts for WGS reactions. They found that defects that reside at the edges of a catalyst's crystalline lattice and, to some extent, the interactions of these defects with the support that they are grown on seem to be critical features governing the WGS activity of these systems. The information gathered from these synchrotron studies can be used to guide the production of cheaper and more efficient catalyst WGS catalysts.

Contact: Christopher Matranga, 412-386-4114

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| 5. | Xingyi Deng, Junseok Lee, Congjun Wang, Christopher Matranga, Funda Aksoy, and Zhi Liu, "In-Situ Observation of Water Dissociation with Lattice Incorporation at FeO Particle Edges Using Scanning Tunneling Microscopy and X-ray Photoelectron Spectroscopy," <i>Langmuir</i> , Vol. 27, 2011, pp 2146-2149. |
| 6. | Kristi L. Kauffman, Jeffrey T. Culp, Angela Goodman, and Christopher Matranga," FT-IR Study of CO_2 Adsorption in a Dynamic Copper(II) Benzoate–Pyrazine Host with CO_2 – CO_2 Interactions in the Adsorbed State," <i>Journal of Physical Chemistry C</i> , Vol. 115, pp 1857-1866. |
| 7. | Yuhua Duan, "Electronic structural and electrochemical properties of lithium zirconates and their capabilities of CO ₂ capture: A first-principles density-functional theory and phonon dynamics approach," <i>Journal of Renewable and Sustainable Energy</i> , 2011, Vol. 3, No.1, pp 013102ff |
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| 10. | Debangsu Bhattacharyya, Richard Turton, and Stephen E. Zitney, "Steady-State Simulation and Optimization of an Integrated Gasification Combined Cycle Power Plant with CO ₂ Capture," Industrial & Engineering Chemistry Research, 2011, 50 (3), pp 1674–1690; DOI: 10.1021/ie101502d. |
| 11. | Ranjani V. Siriwardane, James A. Poston, Jr., Clark Robinson, and Thomas Simonyi, "Effect of additives on decomposition of sodium carbonate: pre-combustion CO ₂ capture sorbent regeneration," <i>Energy Fuels</i> , 2011, 25 (3), pp 1284–1293. |
| 12. | Evgeniy M. Myshakin, Brian J. Anderson, Kelly Rose, and Ray Boswell, Simulations of Variable Bottomhole Pressure Regimes to Improve Production from the Double-Unit Mount Elbert, Milne Point Unit, North Slope Alaska Hydrate Deposit, 2011, pp 1077–1091; DOI: 10.1021/ef101407b. |
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